Dilip Asthagiri

List of Publications by Year
in descending order

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91	3,690	145106	156644
papers	citations	33 h-index	58 g-index

98	98	98	3676
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Comment on â€œCalculation of Solidâ€“Fluid Interfacial Free Energy with Consideration of Solid Deformation by Molecular Dynamicsâ€• Journal of Physical Chemistry A, 2022, 126, 1782-1783.	1.1	1
2	Hydrated Anions: From Clusters to Bulk Solution with Quasi-Chemical Theory. Accounts of Chemical Research, 2022, 55, 2201-2212.	7.6	9
3	Predicting ¹H NMR relaxation in Gd³⁺-aqua using molecular dynamics simulations. Physical Chemistry Chemical Physics, 2021, 23, 20974-20984.	1.3	8
4	Tribute to Lawrence R. Pratt. Journal of Physical Chemistry B, 2021, 125, 4925-4927.	1.2	0
5	Thermodynamics of Hydration from the Perspective of the Molecular Quasichemical Theory of Solutions. Journal of Physical Chemistry B, 2021, 125, 8294-8304.	1.2	9
6	NMR ¹Hâ€“¹H Dipole Relaxation in Fluids: Relaxation of Individual ¹Hâ€“¹H Pairs versus Relaxation of Molecular Modes. Journal of Physical Chemistry B, 2020, 124, 10802-10810.	1.2	8
7	Hydrophilic Interactions Dominate the Inverse Temperature Dependence of Polypeptide Hydration Free Energies Attributed to Hydrophobicity. Journal of Physical Chemistry Letters, 2020, 11, 9965-9970.	2.1	11
8	Insights into the mechanisms affecting water/oil interfacial tension as a function of salt types and concentrations. Fluid Phase Equilibria, 2020, 522, 112771.	1.4	10
9	Toward in silico CMC: An industrial collaborative approach to modelâ€based process development. Biotechnology and Bioengineering, 2020, 117, 3986-4000.	1.7	26
10	Elucidating the ¹H NMR Relaxation Mechanism in Polydisperse Polymers and Bitumen Using Measurements, MD Simulations, and Models. Journal of Physical Chemistry B, 2020, 124, 4222-4233.	1.2	23
11	System Size Dependence of Hydration-Shell Occupancy and Its Implications for Assessing the Hydrophobic and Hydrophilic Contributions to Hydration. Journal of Physical Chemistry B, 2020, 124, 798-806.	1.2	8
12	Critical Role of Confinement in the NMR Surface Relaxation and Diffusion of n-Heptane in a Polymer Matrix Revealed by MD Simulations. Journal of Physical Chemistry B, 2020, 124, 3801-3810.	1.2	23
13	Apolar Behavior of Hydrated Calcite (10Ì…4) Surface Assists in Naphthenic Acid Adsorption. Energy & Fuels, 2019, 33, 6119-6125.	2.5	7
14	Role of internal motions and molecular geometry on the NMR relaxation of hydrocarbons. Journal of Chemical Physics, 2018, 148, 164507.	1.2	28
15	Molecular dynamics simulations of NMR relaxation and diffusion of hydrocarbons. , 2018, , .		3
16	A cluster size distribution theory to study the thermodynamics and phase behavior of multi-bonding single site solutes in patchy colloidal mixtures. Soft Matter, 2018, 14, 7469-7482.	1.2	5
17	NMR spin-rotation relaxation and diffusion of methane. Journal of Chemical Physics, 2018, 148, 204504.	1.2	25
18	Role of Solute Attractive Forces in the Atomic-Scale Theory of Hydrophobic Effects. Journal of Physical Chemistry B, 2018, 122, 6272-6276.	1.2	12

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19	Solvophobic and solvophilic contributions in the water-to-aqueous guanidinium chloride transfer free energy of model peptides. Journal of Chemical Physics, 2018, 148, 222822.	1.2	9
20	Simulation studies of thermodynamic driving forces for the adsorption of naphthenic acid analogues on calcite (1014) surface. , 2018, , .		0
21	Simulation Studies on the Role of Lauryl Betaine in Modulating the Stability of AOS Surfactant-Stabilized Foams Used in Enhanced Oil Recovery. Energy & Fuels, 2017, 31, 1512-1518.	2.5	24
22	Molecular dynamics simulations of NMR relaxation and diffusion of bulk hydrocarbons and water. Journal of Magnetic Resonance, 2017, 277, 15-24.	1.2	59
23	Thermodynamics of mixtures of patchy and spherical colloids of different sizes: A multi-body association theory with complete reference fluid information. Journal of Chemical Physics, 2017, 146, 164904.	1.2	7
24	Mini-grand canonical ensemble: Chemical potential in the solvation shell. Journal of Chemical Physics, 2017, 147, 164901.	1.2	6
25	Electrostatic and induction effects in the solubility of water in alkanes. Journal of Chemical Physics, 2017, 147, 074506.	1.2	5
26	Adsorption and Phase Behavior of Pure/Mixed Alkanes in Nanoslit Graphite Pores: An iSAFT Application. Langmuir, 2017, 33, 11189-11202.	1.6	47
27	Intramolecular Interactions Overcome Hydration to Drive the Collapse Transition of Gly₁₅. Journal of Physical Chemistry B, 2017, 121, 8078-8084.	1.2	26
28	Quasichemical theory and the description of associating fluids relative to a reference: Multiple bonding of a single site solute. Journal of Chemical Physics, 2017, 147, 124505.	1.2	9
29	Structure and thermodynamics of a mixture of patchy and spherical colloids: A multi-body association theory with complete reference fluid information. Journal of Chemical Physics, 2016, 145, 074904.	1.2	16
30	Response to â€œComment on â€˜Isolating the non-polar contributions to the intermolecular potential for water-alkane interactionsâ€â€™ [J. Chem. Phys. 144, 137101 (2016)]. Journal of Chemical Physics, 2016, 144, 137102.	1.2	7
31	Molecular Theory and the Effects of Solute Attractive Forces on Hydrophobic Interactions. Journal of Physical Chemistry B, 2016, 120, 1864-1870.	1.2	25
32	Understanding the Thermodynamics of Hydrogen Bonding in Alcohol-Containing Mixtures: Cross-Association. Journal of Physical Chemistry B, 2016, 120, 3388-3402.	1.2	46
33	Extensions of the SAFT model for complex association in the bulk and interface. Fluid Phase Equilibria, 2016, 416, 62-71.	1.4	10
34	Importance of Hydrophilic Hydration and Intramolecular Interactions in the Thermodynamics of Helixâ€“Coil Transition and Helixâ€“Helix Assembly in a Deca-Alanine Peptide. Journal of Physical Chemistry B, 2016, 120, 69-76.	1.2	26
35	Breast Cancerâ€“Specific miR Signature Unique to Extracellular Vesicles Includes â€œmicroRNA-likeâ€•tRNA Fragments. Molecular Cancer Research, 2015, 13, 891-901.	1.5	84
36	Conditional Solvation Thermodynamics of Isoleucine in Model Peptides and the Limitations of the Group-Transfer Model. Journal of Physical Chemistry B, 2014, 118, 4080-4087.	1.2	15

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37	Polymorphic Protein Crystal Growth: Influence of Hydration and Ions in Glucose Isomerase. Crystal Growth and Design, 2014, 14, 46-57.	1.4	17
38	Solvation Free Energy of the Peptide Group: Its Model Dependence and Implications for the Additive-Transfer Free-Energy Model of Protein Stability. Biophysical Journal, 2013, 105, 1482-1490.	0.2	21
39	Solvation Free Energies of Alanine Peptides: The Effect of Flexibility. Journal of Physical Chemistry B, 2013, 117, 16428-16435.	1.2	27
40	Role of Local Metal-Site Interactions and Bulk Protein Restraints in the Thermodynamics of Zinc Binding to a Zinc Finger Protein. Biophysical Journal, 2012, 102, 457a.	0.2	1
41	Regularizing Binding Energy Distributions and the Hydration Free Energy of Protein Cytochrome C from All-Atom Simulations. Journal of Chemical Theory and Computation, 2012, 8, 3409-3415.	2.3	37
42	Quasi-Chemical Theory of Cosolvent Hydrophobic Preferential Interactions. Journal of Physical Chemistry B, 2012, 116, 6506-6513.	1.2	3
43	Coordination state probabilities and the solvation free energy of Zn2+ in aqueous methanol solutions. Journal of Chemical Physics, 2012, 137, 164504.	1.2	9
44	An Elastic-Network-Based Local Molecular Field Analysis of Zinc Finger Proteins. Journal of Physical Chemistry B, 2011, 115, 7374-7382.	1.2	7
45	The Role of Bulk Protein in Local Models of Ion-Binding to Proteins: Comparative Study of KcsA, Its Semisynthetic Analog with a Locked-in Binding Site, and Valinomycin. Biophysical Journal, 2011, 100, 1542-1549.	0.2	11
46	Separating the Role of Protein Restraints and Local Metal-Site Interaction Chemistry in the Thermodynamics of a Zinc Finger Protein. Biophysical Journal, 2011, 101, 1459-1466.	0.2	2
47	Water coordination structures and the excess free energy of the liquid. Journal of Chemical Physics, 2011, 134, 124514.	1.2	13
48	Communication: Regularizing binding energy distributions and thermodynamics of hydration: Theory and application to water modeled with classical and ab initio simulations. Journal of Chemical Physics, 2011, 135, 181101.	1.2	19
49	Thermodynamics of ion selectivity in the KcsA K+ channel. Journal of General Physiology, 2011, 137, 427-433.	0.9	20
50	Ion-water clusters, bulk medium effects, and ion hydration. Journal of Chemical Physics, 2011, 135, 054505.	1.2	19
51	Ion selectivity from local configurations of ligands in solutions and ion channels. Chemical Physics Letters, 2010, 485, 1-7.	1.2	80
52	Communication: Thermodynamics of water modeled using ab initio simulations. Journal of Chemical Physics, 2010, 133, 141101.	1.2	31
53	Long range interactions in nanoscale science. Reviews of Modern Physics, 2010, 82, 1887-1944.	16.4	359
54	Molecular packing and chemical association in liquid water simulated using ab initio hybrid Monte Carlo and different exchange-correlation functionals. Journal of Chemical Physics, 2010, 132, 204509.	1.2	14

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55	Thermodynamically dominant hydration structures of aqueous ions. Journal of Chemical Physics, 2009, 130, 195102.	1.2	50
56	Ion Selectivity in the KcsA Potassium Channel from the Perspective of the Ion Binding Site. Biophysical Journal, 2009, 96, 2138-2145.	0.2	38
57	Distinguishing Thermodynamic and Kinetic Views of the Preferential Hydration of Protein Surfaces. Biophysical Journal, 2008, 95, 2219-2225.	0.2	13
58	Role of attractive methane-water interactions in the potential of mean force between methane molecules in water. Journal of Chemical Physics, 2008, 128, 244512.	1.2	57
59	Single ion hydration free energies: A consistent comparison between experiment and classical molecular simulation. Journal of Chemical Physics, 2008, 129, 204501.	1.2	31
60	Balancing local order and long-ranged interactions in the molecular theory of liquid water. Journal of Chemical Physics, 2007, 127, 144508.	1.2	42
61	Potential Distribution Methods and Free Energy Models of Molecular Solutions. Springer Series in Chemical Physics, 2007, , 323-351.	0.2	28
62	Non-van der Waals Treatment of the Hydrophobic Solubilities of CF4. Journal of the American Chemical Society, 2007, 129, 10133-10140.	6.6	35
63	Beryllium Displacement of H+ from Strong Hydrogen Bonds. Angewandte Chemie - International Edition, 2007, 46, 2669-2671.	7.2	29
64	Water adsorption and dissociation on BeO(001) and (100) surfaces. Surface Science, 2007, 601, 1608-1614.	0.8	10
65	Role of fluctuations in a snug-fit mechanism of KcsA channel selectivity. Journal of Chemical Physics, 2006, 125, 024701.	1.2	44
66	An analysis of molecular packing and chemical association in liquid water using quasichemical theory. Journal of Chemical Physics, 2006, 124, 224502.	1.2	37
67	Ab initio molecular dynamics and quasichemical study of H+(aq). Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 6704-6708.	3.3	94
68	A Consistent Experimental and Modeling Approach to Light-Scattering Studies of Protein-Protein Interactions in Solution. Biophysical Journal, 2005, 88, 3300-3309.	0.2	48
69	Light-Scattering Studies of Protein Solutions: Role of Hydration in Weak Protein-Protein Interactions. Biophysical Journal, 2005, 89, 1564-1573.	0.2	50
70	From The Cover: Hydration and mobility of HO-(aq). Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 7229-7233.	3.3	145
71	On the Role of the Conserved Aspartate in the Hydrolysis of the Phosphocysteine Intermediate of the Low Molecular Weight Tyrosine Phosphatase. Journal of the American Chemical Society, 2004, 126, 12677-12684.	6.6	22
72	Inner shell definition and absolute hydration free energy of K+(aq) on the basis of quasi-chemical theory and ab initio molecular dynamics. Physical Chemistry Chemical Physics, 2004, 6, 1966-1969.	1.3	88

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73	Hydration Structure and Free Energy of Biomolecularly Specific Aqueous Dications, Including Zn2+ and First Transition Row Metals. Journal of the American Chemical Society, 2004, 126, 1285-1289.	6.6	155
74	Pressure Denaturation of Staphylococcal Nuclease Studied by Neutron Small-Angle Scattering and Molecular Simulation. Biophysical Journal, 2004, 87, 3479-3492.	0.2	75
75	Absolute hydration free energies of ions, ionâ€“water clusters, and quasichemical theory. Journal of Chemical Physics, 2003, 119, 2702-2708.	1.2	200
76	The hydration state of HOâ¯(aq). Chemical Physics Letters, 2003, 380, 530-535.	1.2	59
77	Quasi-chemical study of Be2+(aq) speciation. Chemical Physics Letters, 2003, 371, 613-619.	1.2	57
78	Hydration of krypton and consideration of clathrate models of hydrophobic effects from the perspective of quasi-chemical theory. Biophysical Chemistry, 2003, 105, 323-338.	1.5	45
79	Free energy of liquid water on the basis of quasichemical theory andab initiomolecular dynamics. Physical Review E, 2003, 68, 041505.	0.8	133
80	Quasi-Chemical Theory and the Standard Free Energy of H+(aq). Journal of Physical Chemistry A, 2002, 106, 9145-9148.	1.1	60
81	Density Functional Study of the Mechanism of a Tyrosine Phosphatase:Â I. Intermediate Formation. Journal of the American Chemical Society, 2002, 124, 10225-10235.	6.6	44
82	Continuum and Atomistic Modeling of Ion Partitioning into a Peptide Nanotube. Biophysical Journal, 2002, 82, 1176-1189.	0.2	44
83	Measured and calculated effects of mutations in bacteriophage T4 lysozyme on interactions in solution. Proteins: Structure, Function and Bioinformatics, 2000, 41, 123-132.	1.5	17
84	Role of competitive interactions in growth rate trends of subtilisin s88 crystals. Journal of Crystal Growth, 2000, 212, 543-554.	0.7	11
85	Calculation of Hydration Effects in the Binding of Anionic Ligands to Basic Proteins. Journal of Physical Chemistry B, 2000, 104, 8753-8761.	1.2	19
86	Measured and calculated effects of mutations in bacteriophage T4 lysozyme on interactions in solution. Proteins: Structure, Function and Bioinformatics, 2000, 41, 123-132.	1.5	1
87	Measured and calculated effects of mutations in bacteriophage T4 lysozyme on interactions in solution. Proteins: Structure, Function and Bioinformatics, 2000, 41, 123-32.	1.5	4
88	Calculation of short-range interactions between proteins. Biophysical Chemistry, 1999, 78, 219-231.	1.5	46
89	Why is the osmotic second virial coefficient related to protein crystallization?. Journal of Crystal Growth, 1999, 196, 377-387.	0.7	179
90	Molecular Origins of Osmotic Second Virial Coefficients of Proteins. Biophysical Journal, 1998, 75, 2469-2477.	0.2	254

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91	Influence of Structural Details in Modeling Electrostatically Driven Protein Adsorption. Langmuir, 1997, 13, 6761-6768.	1.6	91